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(FILE 'HOME' ENTERED AT 11:17:55 ON 23 MAR 2007)
FILE 'CA' ENTERED AT 11:19:53 ON 23 MAR 2007
L1 365 S (THERMOCHEM? OR THERMOG? OR THERMOANALY? OR THERMAL ANALY?) AND
(MICROARRAY OR ARRAY OR BIOCHIP OR MICROTIT? OR MICROWELL OR
MULTIWELL OR MICROPLATE OR(96 OR 384 OR 768 OR 1536 OR 3456 OR 9600)
(2A) WELL)
L2 1314 S (THERMOCHEM? OR THERMOG? OR THERMOANALY? OR THERMAL ANALY?) AND
(PHARMACEUT? OR DRUG OR MEDIC?) (2A) (SCREEN? OR TEST? OR EVALUAT? OR
DISCOVER? OR IDENTIF? OR ASSESS? OR MONITOR?) OR COMBINATOR? OR
HYBRIDIZ? OR MOLECUL? (2A) (INTERACT? OR REACT?))
L3 33 S L1 AND L2
L4 29 S L1-2 AND ENZYM?
L5 32 S L1-2 AND (96 OR 384 OR 768 OR 1536 OR 3456 OR 9600)
L6 12 S L1-2 AND EQUILIBRAT?
L7 24 S L1-2 AND MICROCALORIM?
L8 177 S L1-2 AND CALORIMET?
L9 83 S L1-2 AND INFRARED(1A) (IMAG? OR THERMOGR?)
L10 7 S L8 AND INHIBIT?
L11 12 S L9 AND (ENDOTHERM? OR CORRECT? OR CELL FREE OR HOTPLATE OR AGONIST)
L12 132 S L3-7, L10-11
L13 91 S L12 AND PY<2004
L14 26 S L12 AND PATENT/DT
FILE 'BIOSIS' ENTERED AT 12:14:51 ON 23 MAR 2007
L15 24 S L13
FILE 'MEDLINE' ENTERED AT 12:16:17 ON 23 MAR 2007
L16 24 S L13
FILE 'CA, BIOSIS, MEDLINE' ENTERED AT 12:18:41 ON 23 MAR 2007
L17 117 DUP REM L13 L14 L15 L16 (48 DUPLICATES REMOVED)

=> d 117 1-117 bib,ab

L17 ANSWER 12 OF 117 CA COPYRIGHT 2007 ACS on STN
AN 138:278132 CA
TI Infrared spectroscopic imaging of libraries
IN McFarland, Eric W.; Archibald, William
PA Symyx Technologies, Inc., USA
SO U.S., 19 pp., Cont.-in-part of U.S. 6,030,917.
PI US 6541271 B1 20030401 US 1997-946135 19971007
US 6030917 A 20000229 US 1997-898715 19970722
PRAI US 1996-28105P P 19961009
AB Methods of characterizing a relative thermal diffusivity for a plurality of materials are described which entail providing a thermally uniform substrate having a **combinatorial array** comprising a plurality of diverse materials at known locations on a first surface of the substrate; irradiating a second surface of the substrate with an IR source; modulating the IR source; and monitoring a temp. change assocd. with each of the plurality of materials as a function of time, the temp. change indicative of the relative thermal diffusivity of the plurality of materials. Systems for characterizing a relative thermal diffusivity for a plurality of materials are described which comprise a thermally uniform substrate adapted for contg. an **array** of materials on a first surface of the substrate; a modulated IR radiation source for directing

modulated IR radiation at a second surface of the substrate, where the IR radiation is substantially uniform across the plurality of materials; an IR detector **array** for monitoring a temp. change assocd. with each material of the plurality of materials as a function of time, the IR detector adapted for outputting a plurality of signals corresponding to the monitored temp. change for each material; and a processor coupled to the IR detector **array**, where the processor is adapted for recording the output signals from the detector **array** and detg. the relative thermal diffusivity of the plurality of materials.

L17 ANSWER 26 OF 117 CA COPYRIGHT 2007 ACS on STN
AN 137:329829 CA
TI Simultaneous high throughput assessment of thermodynamic and kinetic behaviour of chemical reactions: theory and experiment
AU Davies, Gary C.; Hutton, Roger S.; Millot, Nicolas; Macdonald, Simon J. F.; Anson, Mike S.; Campbell, Ian B.
CS GlaxoSmithKline, Harlow, Essex, CM19 5AW, UK
SO Physical Chemistry Chemical Physics (2002), 4(10), 1791-1796
AB There is an increasing requirement in the pharmaceutical industry to rapidly monitor reactions. High throughput screening (HTS) is typically achieved by performing expts. simultaneously in **array** format in **microtiter** plates. One method of monitoring reactions that has received particular attention recently is the use of thermal measurements. The change in temp. with time resulting from a reaction depends on both thermodn. and kinetics. Temp. can be monitored in a no. of ways, one of which is suitable for HTS is **thermog.** imaging. Relating such thermal information to reaction parameters such as enthalpy and rate is complicated by issues such as heat loss to the surroundings and heat transfer to different parts of the app. A method is presented whereby information obtained from thermal imaging of **microtiter** plates can be used, along with exptl. data for heat transfer to the surroundings and the **microtiter** plate, to rank reaction enthalpy and time to completion of a set of reactions. Finally, a comparison to enthalpies obtained by **microcalorimetry** is made.

L17 ANSWER 28 OF 117 CA COPYRIGHT 2007 ACS on STN
AN 137:41018 CA
TI Rapid determination of enantiomeric excess using infrared **thermography**
AU Millot, Nicolas; Borman, Phil; Anson, Mike S.; Campbell, Ian B.; Macdonald, Simon J. F.; Mahmoudian, Mahmoud
CS Medicines Research Centre, GlaxoSmithKline Research and Development, Hertfordshire, SG1 2NY, UK
SO Organic Process Research & Development (2002), 6(4), 463-470
AB IR **thermog.** (IRT) is presented as a novel technique to screen a potentially large no. of asym. catalysts or substrates in a high-throughput fashion. IRT was used as a simple, rapid, and practical approach for initial screening of the substrate specificity of *Candida antarctica* lipase. This was carried out using a **96-well microtiter** plate format. Potential advantages and limitations of IRT for the **enzymic** stereoselective acylation of primary and secondary alcs. of interest are discussed.

L17 ANSWER 35 OF 117 CA COPYRIGHT 2007 ACS on STN

AN 134:125924 CA
TI Thermochemical sensors and use in pharmaceutical agent screening
IN Connelly, Patrick R.; Ali, Janid Asghar; Bruzzese, Frank Joseph;
Faerman, Carlos H.
PA The Althexis Co., Inc., USA
SO PCT Int. Appl., 98 pp.
PI WO 2001006250 A2 20010125 WO 2000-US19383 20000718
PRAI US 1999-144579P P 19990719
AB Methods are provided to link the binding event of a test ligand or substrate to a target (e.g. a target protein) to the generation of a heat output. The methods can be used to screen for pharmaceutical agents.

L17 ANSWER 40 OF 117 CA COPYRIGHT 2007 ACS on STN
AN 135:163919 CA
TI Infrared-thermographic screening of the activity and enantioselectivity of enzymes
AU Reetz, M. T.; Hermes, M.; Becker, M. H.
CS Max-Planck-Institut fur Kohlenforschung, Mulheim an der Ruhr, 45470, Germany
SO Applied Microbiology and Biotechnology (2001), 55(5), 531-536
AB A review with approx. 50 refs. The IR radiation caused by the heat of reaction of an enantioselective enzyme-catalyzed transformation can be detected by modern photovoltaic IR (IR)-thermog. cameras equipped with focal plane array detectors. Specifically, in the lipase-catalyzed enantioselective acylation of racemic 1-phenylethanol, the (R)- and (S)-substrates are allowed to react sep. in the wells of microtiter plates, the (R)-alc. showing hot spots in the IR-thermog. images. Thus, highly enantioselective enzymes can be identified at kinetic resoln.

L17 ANSWER 43 OF 117 MEDLINE on STN
AN 2001354994 MEDLINE
TI Novel methods for biocatalyst screening.
AU Wahler D; Reymond J L
CS Departement fur Chemie und Biochemie, Universitat Bern, Switzerland.
SO Current opinion in chemical biology, (2001 Apr) Vol. 5, No. 2, pp. 152-8.
AB There have been a number of recent advances in catalysis assays applicable for screening biocatalyst libraries in high-throughput format. These include instrumental assays such as high-performance liquid chromatography, mass spectrometry, capillary electrophoresis and IR-thermography, reagent-based assays producing spectroscopic signals (UV/VIS or fluorescence) in response to reaction progress, and assays based on fluorogenic or chromogenic substrates. These fluorogenic substrates enable the assaying of a variety of enzymes in enantioselective and stereoselective manner, including alcohol dehydrogenases, aldolases, lipases, amidases, epoxide hydrolases and phosphatases.

L17 ANSWER 51 OF 117 CA COPYRIGHT 2007 ACS on STN
AN 133:266394 CA
TI IR-thermographic screening of thermoneutral or endothermic transformations: the ring-closing olefin metathesis reaction

AU Reetz, Manfred T.; Becker, Michael H.; Liebl, Monika; Furstner, Alois
CS Max-Planck-Institut fur Kohlenforschung, Mulheim an der Ruhr, 45470,
Germany
SO Angewandte Chemie, International Edition (2000), 39(7), 1236-1239
AB In appropriate systems **endothermic** or even thermoneutral reactions can
be successfully screened by resolved detection of cold spots in **IR-**
thermog. **images**. This is useful for screening **combinatorial** libraries
of catalysts.

L17 ANSWER 54 OF 117 CA COPYRIGHT 2007 ACS on STN
AN 132:227998 CA
TI Catalytic phenomena in **combinatorial** libraries of heterogeneous
catalysts detection of activation and deactivation by emissivity-
corrected IR thermography
AU Holzwarth, Arnold; Maier, Wilhelm F.
CS Max-Planck-Institut fur Kohlenforschung, Mulheim an der Ruhr, Germany
SO Platinum Metals Review (2000), 44(1), 16-21
AB A review with 13 refs.; **combinatorial** catalysis is becoming a
significant method for investigating the activities of large nos. of
potential catalysts. A very important prerequisite for making use of
combinatorial catalysis research is a reliable, fast and efficient
technique for monitoring the catalytic activities. Emissivity-cor. **IR**
thermog., which monitors the heat changes resulting from the heat of
reaction on catalyst surfaces, is such a technique. In this article we
describe emissivity-cor. **IR** **thermog.** and demonstrate its performance,
over time, in monitoring the catalytic activities of catalyst libraries.
It is shown that not only can static relative activity be displayed, but
also that catalyst-specific time-dependent properties, such as
activation and deactivation phenomena can be demonstrated.

L17 ANSWER 55 OF 117 CA COPYRIGHT 2007 ACS on STN
AN 132:1820 CA
TI **Infrared thermography** for measuring real-time **thermogenesis** in organisms
and cells
IN Lenhard, James Martin; Paulik, Mark Andrew
PA Glaxo Group Limited, UK
SO PCT Int. Appl., 93 pp.
PI WO 9960630 A1 19991125 WO 1999-US10579 19990514
US 6881584 B1 20050419 US 1999-441493 19991117
PRAI US 1998-85736P P 19980515
AB The present invention relates, in general, to **thermog.** and, in
particular, to a method of using **IR** **thermog.** to monitor physiol. and
mol. events that elicit a **thermogenic** response in animals (including
humans), plants, tissues, cells and **cell-free** systems. The present
method can be used for screening, **identifying**, and ranking **drug**
candidates for multiple diseases, disorders and conditions. Three
different inbred strains of mice, AKR/J, C57BL/6J, and SWR/J, were
maintained on high and low fat diets for 14 wk before treatment with the
 β 3-adrenoceptor **agonist**, BRL37344. The heat produced in the
intrascapular region was measured before and after 60 min treatment
using **IR** **thermog.** The obesity prone mice, AKR/J, had a greater
thermogenic response to BRL37344 when fed the higher fat diet. The

obesity resistant mice, SWR/J, had a greater **thermogenic** response when fed the lower fat diet. There was little difference in the response of C57BL/6J mice on a high or low fat diet.

L17 ANSWER 67 OF 117 CA COPYRIGHT 2007 ACS on STN
AN 130:95129 CA
TI Time-resolved IR-**thermographic** detection and screening of enantioselectivity in catalytic reactions
AU Reetz, Manfred T.; Becker, Michael H.; Kuhling, Klaus M.; Holzwarth, Arnold
CS Max-Planck-Institut fur Kohlenforschung, Mulheim an der Ruhr, D-45470, Germany
SO Angewandte Chemie, International Edition (1998), 37(19), 2647-2650
AB Time-resolved IR **thermog.** was applied to screening of enantioselectivity in catalytic reactions,. Since spacial resoln. is not a problem, the screening of large libraries of asym. catalysts could be possible. The method could also be amenable to other chem. or biochem. processes such as mol. recognition in host-guest chem. or antibody-antigen interactions.
RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 68 OF 117 CA COPYRIGHT 2007 ACS on STN
AN 129:307011 CA
TI Detection of catalytic activity in **combinatorial** libraries of heterogeneous catalysts by **IR thermography**
AU Holzwarth, Arnold; Schmidt, Hans-Werner; Maier, Wilhelm F.
CS Max-Planck-Institut fur Kohlenforschung, Mulheim an der Ruhr, D-45470, Germany
SO Angewandte Chemie, International Edition (1998), 37(19), 2644-2647
AB The primary interest of this study was to display temp. differences due to catalytic activity on a library of heterogeneous catalysts. This was achieved by applying a linear **correction** to the detector response and subtracting the **IR image** of the library just before the start of the reaction as background (offset) from the images during an isothermal catalytic expt. We have demonstrated that, after careful removal of artifacts, **IR imaging** is a powerful tool for the detection of catalytic activities on **combinatorial** libraries. Temp. differences down to 0.1 K can reliably be detected and the heat evolution of catalyzed gas-phase reactions on small catalyst amts. (<20 μ g) identified. Reactions have been obsd. at temps. up to 350°C, indicating that the method can be applied over a wide temp. range.

L17 ANSWER 69 OF 117 CA COPYRIGHT 2007 ACS on STN
AN 129:117364 CA
TI Development of **infrared imaging** to measure **thermogenesis** in cell culture: **thermogenic** effects of uncoupling protein-2, troglitazone, and β -adrenoceptor **agonists**
AU Paulik, Mark A.; Buckholz, Richard G.; Lancaster, Mary E.; Dallas, Walter S.; Hull-Ryde, Emily A.; Weiel, James E.; Lenhard, James M.
CS Department of Metabolic Diseases, GlaxoWellcome Inc. Research Triangle Park, NC, 27709, USA
SO Pharmaceutical Research (1998), 15(6), 944-949

AB Although the effects of **thermogenic** agents in cell culture can be measured by direct **microcalorimetry**, only a few samples can be analyzed over several hours. In this report, we describe a robust non-invasive technique to measure real-time **thermogenesis** of cells cultured in **microtiter** plates using **IR thermog.** Yeast were transformed with uncoupling protein-2 (UCP2) or exposed to carbonyl cyanide p-(trifluoromethoxy)phenylhydrazone (FCCP) or rotenone. Adipocytes were exposed to rotenone, FCCP, cycloheximide, troglitazone, or CL316243. **Thermogenesis** was measured using **IR thermog.** **Thermogenesis** increased after exposing yeast to the mitochondrial uncoupler, FCCP, or transforming the cells with UCP2. Further, **thermogenesis** in adipocytes was stimulated by CL316243, a β 3-adrenoceptor **agonist** being developed to treat obesity. The protein synthesis inhibitor, cycloheximide, did not inhibit CL316243-mediated **thermogenesis**. In contrast, the mitochondrial proton transport inhibitor, rotenone, inhibited **thermogenesis** in yeast and adipocytes. Similarly, the antidiabetic agent, troglitazone, suppressed **thermogenesis** in adipocytes. Although increased UCP synthesis resulted in increased **thermogenesis** in yeast, UCP expression did not correlate with **thermogenesis** in adipocytes. The results, taken together with the high resoln. (0.002°C) and robustness (384-well format) of the approach, indicate **IR-imaging** is a rapid and effective method for measuring **thermogenesis** in vitro.

L17 ANSWER 77 OF 117 CA COPYRIGHT 2007 ACS on STN
AN 127:250453 CA
TI Catalyst testing process and apparatus
IN Willson, Richard Coale, III
PA Technology Licensing Co. L.L.C., USA; Willson, Richard Coale, III
SO PCT Int. Appl., 35 pp.
PI WO 9732208 A1 19970904 WO 1997-US2756 19970225
US 6063633 A 20000516 US 1996-664836 19960617
PRAI US 1996-12457P P 19960228
AB A multicell holder, e.g., a honeycomb or plate, or a collection of individual support particles, is treated with solns./suspensions of catalyst ingredients to produce a plurality of cells, spots, or pellets each having a different compn. The plurality of cells, spots, or pellets are dried, calcined or treated to stabilize the ingredients and contacted with a potentially reactive feed stream or batch of reactants. The reaction occurring in each cell is measured or analyzed to det. the relative efficacy of the catalysts in each combination. The measurement or anal. is done through a no. of different methods including **IR thermog.**, spectroscopy of products or residual reactants or sampling for further anal. Robotic techniques can be employed in producing the cells, spots or pellets.

L17 ANSWER 96 OF 117 CA COPYRIGHT 2007 ACS on STN
AN 119:240815 CA
TI Application of **microcalorimetric** technique for the screening and examination of medicines
AU Zhang, Youmin; Wang, Baohuai
CS Inst. Phys. Chem., Beijing Univ., Beijing, 100871, Peop. Rep. China
SO Journal of Chinese Pharmaceutical Sciences (1993), 2(1), 24-32
AB According to the heating effect caused by interaction between matters, a

series of expts. on the interaction between drugs and cells from human bodies, DNA and physiol. saline have been carried out with MS-80 std. Calvet **microcalorimeter**. The expts. include: (1) thermokinetic studies of the effect of anticancer drugs [sodium norcantharidate (ASN), the bioactive material (Sp.P and Sp.S) from algae etc.] on cancer cells [HeLa, human breast carcinoma)Bcap-37), human adenocarcinoma gastric cells (SGc-7901 and MCF-7) etc.] and the normal cells from human bodies [diploid fibroblasts from human fetal lung (2BS) etc.] at 310.15 K; (2) studies of the intercalation binding of some alkaloidal drugs with the bioactivity to **inhibit** monoamine oxidase (harmaline and harmine etc.) to calf thymus DNA in neutral aq. soln. at 298.15 K; (3) studied of the interaction between long acting drugs (long acting oral contraceptive-norgestrel etc.) and slow-releasing drug (Contac) and aq. soln. of 0.9% NaCl at 310.15 K. All the exptl. results have given their characteristic **thermograms** and the interaction enthalpy changes. On the anal. of all the results, the authors put forward a method on application of **microcalorimetric** technique for screening and examn. of medicines. The principle of application and the exptl. operation of this method have been expounded, and some results of the above expts. have been discussed. As one of the methods for **screening** and examg. **medicines**, the **microcalorimetric** method has some distinguished features and advantages over other methods.

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